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On The Stable Numerical Evaluation of Caputo Fractional Derivatives

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Abstract—The computation of Caputo's fractional derivatives in the presence of measured data is considered as an ill-posed problem and treated by mollification techniques. It is shown that, with the appropriate choice of the radius of mollification, the method is a regularizing algorithm, and the order of convergence is derived. Error estimates are included together with numerical examples of interest. © 2006 Elsevier Ltd. All rights reserved.

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1. INTRODUCTION

Fractional derivatives and partial fractional derivatives have been applied recently to the numerical solution of problems in fluid and continuum mechanics [1], viscoelastic and viscoplastic flow [2], and anomalous diffusion (superdiffusion, non-Gaussian diffusion) [3,4]. Numerous citations to several other applications of fractional derivatives to problems in physics, finance, and hydrology can also be found in these articles.

The usual formulation of the fractional derivative, given in standard references such as [5–7], is the Riemann-Liouville definition.

The Riemann-Liouville fractional derivative of order $\alpha > 0$, of an integrable function g defined on the interval $[0, T]$, is given by the convolution integral,

$$\left(D^{(\alpha)}g\right)(t) = \frac{1}{\Gamma(n-\alpha)}\frac{d^n}{dt^n}\int_0^t \frac{g(s)}{(t-s)^{\alpha+1-n}}\,ds, \qquad 0 \le t \le T, \quad n-1 < \alpha < n, \quad n \in N,$$
$$\left(D^{(\alpha)}g\right)(t) = \frac{d^n g(t)}{dt^n}, \qquad 0 \le t \le T, \quad \alpha = n,$$

where $\Gamma(.)$ is the Gamma function and N indicates the set of natural numbers.

This definition leads to fractional differential equations which require the initial conditions to be expressed not in terms of the solution itself but rather in terms of its fractional derivatives,

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which are difficult to derive from a physical system. In applications, it is often more convenient to use the formulation of the fractional derivative suggested by Caputo [8] which requires the same starting conditions as an ordinary differential equation of order n.

The Caputo fractional derivative of order $\alpha > 0$, of a differentiable function g defined on the interval $[0, T]$, is given by the convolution integral,

$$\left(D^{(\alpha)}g\right)(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{g^{(n)}(s)}{(t-s)^{\alpha+1-n}}\, ds, \qquad 0 \le t \le T, \quad n-1 < \alpha < n, \quad n \in N,$$

$$\left(D^{(\alpha)}g\right)(t) = \frac{d^n g(t)}{dt^n}, \qquad 0 \le t \le T, \quad \alpha = n.$$

One important difference between the Caputo fractional derivative and the Riemann-Liouville fractional derivative, besides the different requirements on the function g itself, is that the Caputo derivative of a constant is zero. For further details and relationships between these two types of fractional derivatives as well as a historical perspective on fractional derivatives in general, see [5].

Fractional differential operators are particular first-kind Volterra integral equations (nonlocal operators) with weakly singular kernels and the above formulations are of little use in practice unless the data is known exactly.

The purpose of this paper is to present and analyze a stable method, based on mollification techniques, for the numerical computation of Caputo fractional derivatives when the data function $g^{(n-1)}$ is measured with noise.

The manuscript is organized as follows. In Section 2, the original ill-posed problem and the associated regularized (mollified) problem, respectively, are formulated. The numerical procedure, together with the stability and error analysis of the algorithm are investigated in Section 3. Numerical examples are also provided in this section. In the Appendix (Section 4), for completeness, we state basic properties and estimates corresponding to mollification in $\mathbf{R}^1$.

2. BACKGROUND AND REGULARIZATION

In this section, we utilize the notation and concepts introduced in the Appendix (Section 4). Without loss of generality, we restrict our attention to functions defined on the interval $I = [0, 1]$ and consider the case $n = 1$.

We would like to determine the Caputo fractional derivative of order α,

$$\left(D^{(\alpha)}g\right)(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{g'(s)}{(t-s)^{\alpha}}\, ds, \qquad 0 \le t \le 1, \quad 0 < \alpha < 1, \tag{2.1}$$

from noisy data $g^{\epsilon}(t)$, a perturbed version of the exact data function $g(t)$.

Equation (2.1) is a convolution integral equation that can also be expressed as

$$D^{(\alpha)}g = k * g',$$

where the kernel function k is given by

$$k(t) = \begin{cases} \dfrac{t^{-\alpha}}{\Gamma(1-\alpha)}, & t > 0, \\ 0, & t \le 0. \end{cases}$$

Instead of recovering $D^{(\alpha)}g$, in the presence of noise in the data, we look for a mollified solution $J_\delta(D^{(\alpha)}g^{\varepsilon})$ obtained from the previous equation by convolution with the Gaussian kernel ρ_δ defined in (4.1). Consequently, instead of equation (2.1), we have

$$\begin{aligned} J_\delta\left(D^{(\alpha)}g^{\varepsilon}\right) &= D^{(\alpha)}g^{\varepsilon} * \rho_\delta \\ &= k * (g^{\varepsilon} * \rho_\delta)' \\ &= k * (J_\delta g^{\epsilon})'. \end{aligned}$$

That is, the mollified integral formula becomes, after suitable extension of the data function (Appendix, Section 4.1),

$$J_{\delta}\left(D^{(\alpha)} g^{\epsilon}\right)(t)=\frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{\left(J_{\delta} g^{\epsilon}\right)^{\prime}(s)}{(t-s)^{\alpha}} d s. \tag{2.2}$$

Now, we prove the main properties of the method.

THEOREM 2.1. *If the functions g' and g^{ϵ} are uniformly Lipschitz on I and $\|g-g^{\epsilon}\|_{\infty,I} \leq \epsilon$, then there exists a constant C, independent of δ, such that*

$$\left\|J_{\delta}\left(D^{(\alpha)} g^{\epsilon}\right)-D^{(\alpha)} g\right\|_{\infty, I} \leq \frac{C}{(1-\alpha) \Gamma(1-\alpha)}\left(\delta+\frac{\epsilon}{\delta}\right).$$

PROOF.

(1) For $t \in I$, considering exact data in equations (2.1) and (2.2),

$$\begin{aligned}
\left|\left(D^{(\alpha)} g\right)(t)-J_{\delta}\left(D^{(\alpha)} g\right)(t)\right| &\leq \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t}\left|g^{\prime}(s)-\left(\rho_{\delta} * g\right)^{\prime}(s)\right|(t-s)^{-\alpha} d s \\
&\leq \frac{1}{\Gamma(1-\alpha)}\left\|g^{\prime}-\left(\rho_{\delta} * g\right)^{\prime}\right\|_{\infty, I} \int_{0}^{t}(t-s)^{-\alpha} d s \\
&=\frac{1}{(1-\alpha) \Gamma(1-\alpha)}\left\|g^{\prime}-\left(\rho_{\delta} * g\right)^{\prime}\right\|_{\infty, I} \\
&\leq \frac{C}{(1-\alpha) \Gamma(1-\alpha)} \delta,
\end{aligned}$$

from Theorem 4.1 (Appendix, Section 4.1).

(2) For $t \in I$, considering exact and noisy data in equation (2.2),

$$\begin{aligned}
\left|J_{\delta}\left(D^{(\alpha)} g\right)(t)-J_{\delta}\left(D^{(\alpha)} g^{\epsilon}\right)(t)\right| &\leq \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t}\left|\left(\rho_{\delta} * g\right)^{\prime}(s)-\left(\rho_{\delta} * g^{\epsilon}\right)^{\prime}(s)\right|(t-s)^{-\alpha} d s \\
&\leq \frac{1}{\Gamma(1-\alpha)}\left\|J_{\delta} g^{\prime}-\left(J_{\delta} g^{\epsilon}\right)^{\prime}\right\|_{\infty, I} \int_{0}^{t}(t-s)^{-\alpha} d s \\
&=\frac{1}{(1-\alpha) \Gamma(1-\alpha)}\left\|J_{\delta} g^{\prime}-\left(J_{\delta} g^{\epsilon}\right)^{\prime}\right\|_{\infty, I} \\
&\leq \frac{1}{(1-\alpha) \Gamma(1-\alpha)} \frac{\epsilon}{\delta},
\end{aligned}$$

from Theorem 4.1 (Appendix, Section 4.1).

The final estimate follows from the triangle inequality and the results in Parts (1) and (2).

Stability is valid for each fixed $\delta > 0$ and the optimal rate of convergence is obtained by choosing $\delta = O(\sqrt{\epsilon})$.

The mollified Caputo fractional derivative, reconstructed from noisy data, tends uniformly to the exact solution as $\epsilon \to 0$, $\delta = \delta(\epsilon) \to 0$. This establishes the consistency, stability, and convergence properties of the procedure.

2.1. Abstract Algorithm

The abstract algorithm based on the stable formula (2.2) is as follows.

1. Compute $J_{\delta} g^{\epsilon}$ (this automatically provides $\delta = \delta(\epsilon)$).
2. Evaluate the derivative $(J_{\delta} g^{\epsilon})'$ of the mollified data function $J_{\delta} g^{\epsilon}$.
3. Use a quadrature formula to estimate $J_{\delta}(D^{(\alpha)} g)$ from equation (2.2).

3. NUMERICAL PROCEDURE AND IMPLEMENTATION

To numerically approximate $J_\delta(D^{(\alpha)}g)$, a quadrature formula for the convolution equation (2.2) is needed. The objective is to introduce a simple quadrature and avoid any artificial smoothing in the process. To that effect, we consider a uniform partition K of the interval $I = [0,1]$, with elements $t_i = (i-1)\Delta t$, $i = 1,\dots,n$, $n\Delta t = 1$ and, after the noisy data function G^ε has been suitable extended and the radius of mollification automatically selected (see Appendix, Sections 4.4.1 and 4.4.2), we define a piecewise constant interpolant of the corresponding mollified numerical derivative given by

$$(J_\delta l^\varepsilon)'(t) = \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)\varphi_1(t) + \sum_{i=2}^{j-1}\mathbf{D}_0(J_\delta G^\varepsilon)(t_i)\varphi_i(t) + \mathbf{D}_+(J_\delta G^\varepsilon)(t_j)\varphi_j(t), \qquad 0 \le t \le t_j,$$

where

$$\varphi_1(t) = \begin{cases} 1, & \text{if } 0 \le t \le \dfrac{\Delta t}{2}, \\ 0, & \text{otherwise}, \end{cases}$$

$$\varphi_j(t) = \begin{cases} 1, & \text{if } t_j - \dfrac{\Delta t}{2} \le t \le t_j, \\ 0, & \text{otherwise}, \end{cases}$$

$$\varphi_i(t) = \begin{cases} 1, & \text{if } t_i - \dfrac{\Delta t}{2} \le t \le t_i + \dfrac{\Delta t}{2}, \\ 0, & \text{otherwise}, \end{cases} \qquad i = 2,3,\dots,j-1,$$

and $\mathbf{D}_+$ and $\mathbf{D}_0$ represent the forward and centered finite difference approximations, respectively, to $(J_\delta G^\varepsilon)'$.

The discrete computed solution, denoted $(D^{(\alpha)}G^\varepsilon)_\delta$, is then obtain with the quadrature formula

$$\left(D^{(\alpha)}G^\varepsilon\right)_\delta(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{(J_\delta l^\varepsilon)'(s)}{(t-s)^\alpha}\,ds, \tag{3.1}$$

which, when restricted to the grid points, gives

$$\begin{aligned} \left(D^{(\alpha)}G^\varepsilon\right)_\delta(t_1) &= \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)W_1, \\ \left(D^{(\alpha)}G^\varepsilon\right)_\delta(t_2) &= \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)W_1 + \mathbf{D}_+(J_\delta G^\varepsilon)(t_2)W_2, \\ \left(D^{(\alpha)}G^\varepsilon\right)_\delta(t_j) &= \mathbf{D}_+(J_\delta G^\varepsilon)(t_1)W_1 + \sum_{i=2}^{j-1}\mathbf{D}_0(J_\delta G^\varepsilon)(t_i)W_{j-i+1} \\ &\quad + \mathbf{D}_+(J_\delta G^\varepsilon)(t_j)W_j, \qquad j = 3,\cdots,n. \end{aligned} \tag{3.2}$$

Here the quadrature weights $W_j = W_j(\alpha,\Delta t)$ are integrated exactly with values

$$\begin{aligned} W_1 &= \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\left(\frac{\Delta t}{2}\right)^{1-\alpha}, \\ W_i &= \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\left[\left((2i+1)\frac{\Delta t}{2}\right)^{1-\alpha} - \left((2i-1)\frac{\Delta t}{2}\right)^{1-\alpha}\right], \qquad i = 2,3,\dots,j-1, \end{aligned}$$

and

$$W_j = \frac{1}{\Gamma(1-\alpha)}\frac{1}{1-\alpha}\left[j\Delta t - \left[\left(j-\frac{1}{2}\right)\Delta t\right]^{1-\alpha}\right].$$

The error analysis is discussed next.

THEOREM 3.1. *If the functions g' and g^ϵ are uniformly Lipschitz on I and G and G^ε, the discrete versions of g and g^ε, respectively, satisfy $\|G - G^\epsilon\|_{\infty,K} \le \epsilon$, then*

$$\left\| J_\delta(D^{(\alpha)} g^\varepsilon) - (D^{(\alpha)} G^\varepsilon)_\delta \right\|_{\infty,K} \le \frac{C\,\Delta t}{\Gamma(1-\alpha)(1-\alpha)}.$$

PROOF. The smoothness of $\mathbf{D}(J_\delta G^\epsilon)$ ensures the relationships,

$$\mathbf{D}(J_\delta G^\epsilon) = (J_\delta l^\varepsilon)' + O(\Delta t), \qquad 0 \le t \le 1,$$

and

$$\mathbf{D}(J_\delta G^\epsilon) = (J_\delta g^\epsilon)' + O(\Delta t), \qquad 0 \le t \le 1.$$

Hence,

$$\|(J_\delta l^\varepsilon)' - (J_\delta g^\epsilon)'\|_{\infty,K} \le C\Delta t. \tag{3.3}$$

Subtracting equation (2.2) from equation (3.1) and using (3.3),

$$\left(D^{(\alpha)} G^\varepsilon\right)_\delta (t) - J_\delta\left(D^{(\alpha)} g^\varepsilon\right)(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{(J_\delta l^\varepsilon)'(s) - (J_\delta g^\epsilon)'(s)}{(t-s)^\alpha}\, ds,$$

$$\begin{aligned}\left|\left(D^{(\alpha)} G^\varepsilon\right)_\delta (t) - J_\delta\left(D^{(\alpha)} g^\varepsilon\right)(t)\right| &\le \frac{\|(J_\delta l^\varepsilon)'(s) - (J_\delta g^\epsilon)'\|_{\infty,K}}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-s)^\alpha}\, ds \\ &\le \frac{C\Delta t}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-s)^\alpha}\, ds.\end{aligned}$$

The thesis follows after completing the integration.

COROLLARY 3.2. *Under the hypothesis of Theorems 2.1 and 3.1,*

$$\left\|\left(D^{(\alpha)} G^\varepsilon\right)_\delta - D^{(\alpha)} g\right\|_{\infty,K} \le \frac{C}{\Gamma(1-\alpha)(1-\alpha)}\left(\delta + \frac{\epsilon}{\delta} + \Delta t\right).$$

The error estimate for the discrete case is obtained by adding the global truncation error to the error estimate of the nondiscrete case.

3.1. Numerical Results

In this section, we discuss some numerical tests performed with the algorithm introduced in the previous sections.

The discretization parameters are as follows: the number of time divisions is n, $\Delta t = 1/(n-1)$ and $t_i = (i-1)\Delta t$, $i = 1, 2, \dots, n$.

The use of the average perturbation value ε is only necessary for the purpose of generating the noisy data for the simulations. The filtering procedure automatically adapts the regularization parameter to the quality of the data (Appendix, Section 4.4.2).

Discretized measured approximations of the data are simulated by adding random errors to the exact data functions. Specifically, for an exact data function g, its discrete noisy version is

$$G^\epsilon(t_i) = g(t_i) + \varepsilon_i, \qquad |\varepsilon_i| \le \varepsilon, \quad i = 1, 2, \dots, n,$$

where the $(\varepsilon_i)'$ are Gaussian random variables with variance $\sigma^2 = \varepsilon^2$.

In order to test the stability and accuracy of the algorithm, we consider two examples and a selection of average noise perturbations. The fractional derivative errors are measured by the relative weighted l^2-norms defined by

$$\frac{\left[(1/n)\sum\limits_{n=1}^{n} \left|\left(D^{(\alpha)} G^\varepsilon\right)_\delta (t_i) - D^{(\alpha)} g(t_i)\right|^2\right]^{1/2}}{\left[(1/n)\sum\limits_{n=1}^{n} \left|D^{(\alpha)} g(t_i)\right|^2\right]^{1/2}}.$$

In the examples that follow, we observe that $1/\sqrt{\pi}\ D^{(0.5)}g$ is the Abel's transform of g and also that $D^{(0.99)}g$ can be interpreted as an approximation to the ordinary derivative g'.

EXAMPLE 1. The exact data in this example is provided by the identity function $g(t) = t$, $0 \le t \le 1$. The exact Caputo fractional derivatives are given by

$$D^{(\alpha)}g(t) = \frac{1}{\Gamma(1-\alpha)} \frac{t^{1-\alpha}}{1-\alpha}, \qquad 0 < \alpha < 1, \quad 0 \le t \le 1.$$

The relative errors in the approximation of the fractional derivatives as functions of the amount of noise in the data are shown in Table 1. A graphical illustration of the exact and computed fractional derivatives appears in Figure 1.

Table 1. Relative fractional derivative errors as functions of ϵ for $\alpha = 0.25, 0.50, 0.75, 0.99$ and parameters $p = 3$ and $\Delta t = 1/256$.

Relative l^2-Norm Fractional Derivative Errors				
ε	$\alpha = 0.25$	$\alpha = 0.50$	$\alpha = 0.75$	$\alpha = 0.99$
0.00	0.00229	0.00410	0.01484	0.05906
0.05	0.00161	0.00663	0.01589	0.05993
0.10	0.00169	0.00626	0.01616	0.06040

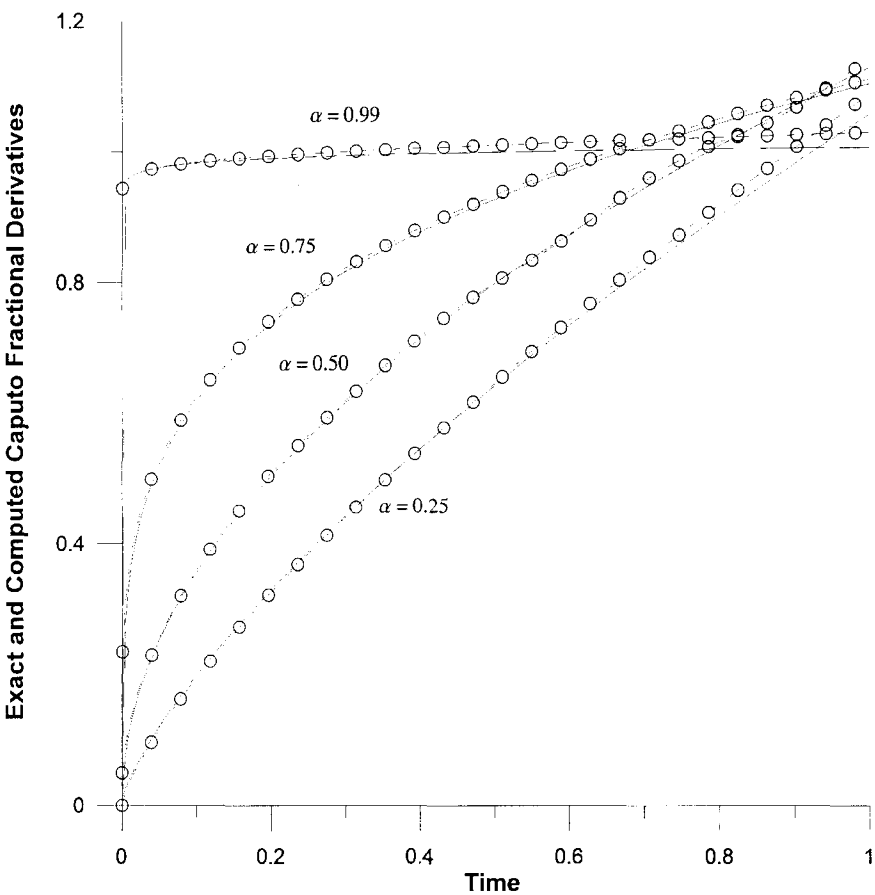

Figure 1. Exact (—) and computed (- o -) fractional derivative functions for $\alpha = 0.25, 0.50, 0.75, 0.99$ and parameters $p = 3$, $\Delta t = 1/256$, and $\varepsilon = 0.1$.

EXAMPLE 2. The exact data function and Caputo fractional derivatives are, respectively, $g(t) = t^2$ and

$$\frac{\Gamma(3)}{\Gamma(3-\alpha)} t^{2-\alpha}, \qquad 0 < \alpha < 1, \quad 0 \le t \le 1.$$

The relative errors in the approximation of the fractional derivatives as functions of the amount of noise in the data are shown in Table 2. A graphical illustration of the exact and computed fractional derivatives is provided in Figure 2.

In all cases, stability with respect to perturbations in the data has been restored and the physical quality of the numerical reconstructions is quite acceptable even in the presence of relatively large amounts of noise in the data. As α increases, the problems become more ill-posed, and for each noise level the relative erors increase accordingly, as expected.

Table 2. Relative fractional derivative errors as functions of ϵ for $\alpha = 0.25, 0.50, 0.75, 0.99$ and parameters $p = 3$ and $\Delta t = 1/256$.

Relative l^2-Norm Fractional Derivative Errors				
ε	$\alpha = 0.25$	$\alpha = 0.50$	$\alpha = 0.75$	$\alpha = 0.99$
0.00	0.00426	0.00603	0.00831	0.00948
0.05	0.00334	0.00891	0.01052	0.01482
0.10	0.00745	0.01413	0.02249	0.06687

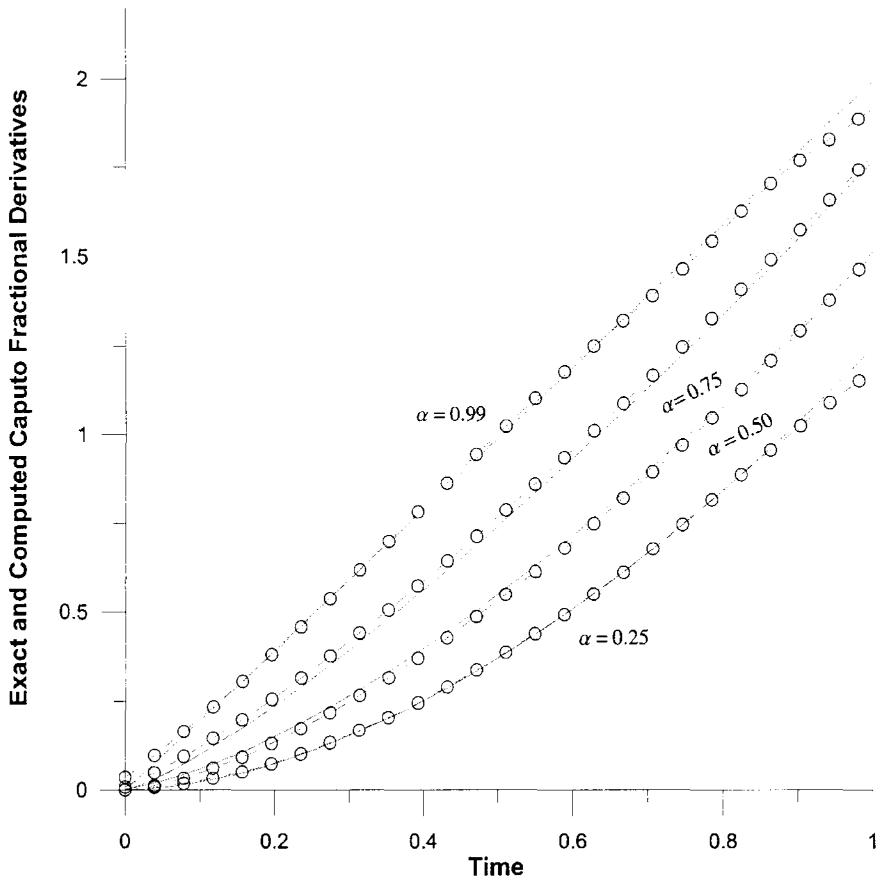

Figure 2. Exact (—) and computed (- o -) fractional derivative functions for $\alpha = 0.25, 0.50, 0.75, 0.99$ and parameters $p = 3$, $\Delta t = 1/256$, and $\varepsilon = 0.1$.

4. APPENDIX

4.1. Mollification

Let $\delta > 0$, $p > 0$ and

$$A_p = \left(\int_{-p}^{p} \exp\left(-s^2\right) \, ds \right)^{-1}.$$

The δ-mollification of an integrable function is based on a convolution with the kernel

$$\rho_{\delta,p}(t) = \begin{cases} A_p \delta^{-1} \exp\left(-\dfrac{t^2}{\delta^2}\right), & |t| \le p\delta, \\ 0, & |t| > p\delta. \end{cases} \tag{4.1}$$

The δ-mollifier $\rho_{\delta,p}$ is a nonnegative $C^\infty(-p\delta, p\delta)$ function satisfying $\int_{-p\delta}^{p\delta} \rho_{\delta,p}(t)\, dt = 1$ and δ is called the radius of mollification. For notational purposes, we will denote the Gaussian kernel by ρ_δ, dropping the dependence on the parameter p.

We set $I = [0,1]$ and $I_\delta = [p\delta, 1 - p\delta]$. Notice that the interval I_δ is nonempty whenever $p < 1/2\delta$.

If f is a locally integrable function on I, we define its δ-mollification on I_δ by the convolution,

$$\begin{aligned} J_\delta f\,(t) &= (\rho_\delta * f)\,(t) \\ &= \int_{-\infty}^{\infty} \rho_\delta\,(t-s)\, f\,(s)\; ds \\ &= \int_{t-p\delta}^{t+p\delta} \rho_\delta\,(t-s)\, f\,(s)\; ds. \end{aligned}$$

The δ-mollification satisfies the following well known consistency and stability estimates. The proofs of the statements in this section can be found in [9].

THEOREM 4.1. CONSISTENCY, STABILITY, AND CONVERGENCE OF MOLLIFICATION. *If f' and f^ϵ are uniformly Lipschitz on I and $\|f - f^\epsilon\|_{\infty,I} \le \epsilon$, then there exists a constant C, independent of δ, such that*

$$\begin{aligned} \|J_\delta f - f\|_{\infty,I_\delta} &\le C\delta, \\ \|J_\delta f - J_\delta f^\epsilon\|_{\infty,I_\delta} &\le \epsilon, \\ \|J_\delta f^\epsilon - f\|_{\infty,I_\delta} &\le C\delta + \epsilon, \end{aligned}$$

and

$$\|(J_\delta f^\epsilon)' - f'\|_{\infty,I_\delta} \le C\left(\delta + \frac{\epsilon}{\delta}\right).$$

4.2. Discrete Mollification

Introduce the set $K = \{t_j : j \in Z,\ 1 \le j \le M\} \subset I$, satisfying

$$t_{j+1} - t_j > d > 0, \qquad j \in Z,$$

and

$$0 \le t_1 < t_2 < \cdots < t_M \le 1,$$

where Z is the set of integers and d is a positive constant. Let $G = \{g_j\}_{j \in Z}$ be a discrete function defined on K, and let $s_j = (1/2)(t_j + t_{j+1})$, $j \in Z$. The discrete δ-mollification of G is defined by

$$J_\delta G(t) = \sum_{j=1}^{M} \left(\int_{s_{j-1}}^{s_j} \rho_\delta(t-s)\, ds \right) g_j .$$

Notice that

$$\sum_{j=1}^{M} \left(\int_{s_{j-1}}^{s_j} \rho_\delta(t-s)\, ds \right) = \int_{-p\delta}^{p\delta} \rho_\delta(s)\, ds = 1.$$

Let

$$\Delta t = \sup_{j \in Z} (t_{j+1} - t_j) .$$

Results of the consistency, stability, and convergence of discrete δ-mollification are as follows.

THEOREM 4.2. CONSISTENCY, STABILITY, AND CONVERGENCE OF DISCRETE MOLLIFICATION.

(1) *If g' is continuous on I and $G = \{g_j = g(t_j) : j \in Z\}$ is the discrete version of g, then there exists a constant C, independent of δ, such that*

$$\|J_\delta G - g\|_{\infty, I_\delta} \le C\,(\delta + \Delta t) ,$$

and

$$\left\|(J_\delta G)' - g'\right\|_{\infty, I_\delta} \le C \left(\delta + \frac{\Delta t}{\delta} \right) .$$

(2) *If g' is continuous on I and the discrete functions,*

$$G = \{g_j : j \in Z\}$$

and

$$G^\epsilon = \{g_j^\epsilon : j \in Z\},$$

which are defined on K, satisfy $\|G - G^\epsilon\|_{\infty, K} \le \epsilon$, then

$$\|J_\delta G - J_\delta G^\epsilon\|_{\infty, I_\delta} \le \epsilon,$$

$$\|(J_\delta G)' - (J_\delta G^\epsilon)'\|_{\infty, I_\delta} \le \frac{C\epsilon}{\delta},$$

$$\|J_\delta G^\epsilon - J_\delta g\|_{\infty, I_\delta} \le C\,(\epsilon + \Delta t) ,$$

$$\|J_\delta G^\epsilon - g\|_{\infty, I_\delta} \le C\,(\epsilon + \delta + \Delta t) ,$$

$$\|(J_\delta G^\epsilon)' - (J_\delta g)'\|_{\infty, I_\delta} \le \frac{C}{\delta}\,(\epsilon + \Delta t) ,$$

and

$$\|(J_\delta G^\epsilon)' - g'\|_{\infty, I_\delta} \le C \left(\delta + \frac{\epsilon}{\delta} + \frac{\Delta t}{\delta} \right) .$$

4.3. Numerical Differentiation

The mollification technique described in the previous sections can be used to obtain a stable reconstruction of the derivative of a function which is known approximately at a discrete set of data points.

In order to recover the derivative g' from discrete noisy data, instead of utilizing $\frac{d}{dt}\rho_\delta$ and convolution with the data, computations are performed with a centered difference approximation of the mollified derivative $\frac{d}{dt}J_\delta G^\epsilon$. Denoting the centered difference operator by $\mathbf{D}$, i.e.,

$$\mathbf{D}f(x) = \frac{f(t+\Delta t) - f(t-\Delta t)}{2\Delta t},$$

we have the following.

THEOREM 4.3. *If g' is continuous on R^1, and*

$$G = \{g_j = g(t_j) : j \in Z\}$$

is the discrete version of g, with G, G^ϵ satisfying

$$\|G - G^\epsilon\|_{\infty,K} \le \epsilon,$$

then

$$\|\mathbf{D}(J_\delta G^\epsilon) - (J_\delta g)'\|_\infty \le \frac{C}{\delta}(\epsilon + \Delta t) + C_\delta (\Delta t)^2$$

and

$$\|\mathbf{D}(J_\delta G^\epsilon) - g'\|_\infty \le C\left(\delta + \frac{\epsilon}{\delta} + \frac{\Delta t}{\delta}\right) + C_\delta(\Delta t)^2.$$

Generally, if

$$G = \{g_j : j \in Z\}$$

is a discrete function defined on K, we define a differentiation operator $\mathbf{D}_0^\delta$ by the following rule,

$$\mathbf{D}_0^\delta(G) = \mathbf{D}\left.(J_\delta G)\right|_K.$$

The next theorem states a useful bound for this operator.

THEOREM 4.4.

$$\left\|\mathbf{D}_0^\delta(G)\right\|_{\infty,K} \le \frac{C}{\delta}\|G\|_{\infty,K}.$$

4.4. Implementation

In most applications, the data functions are given in finite intervals. The mollification of such functions have been discussed extensively in [9,10] and more recently in [11].

4.4.1. Extension of data

Computation of $J_\delta g$ and $J_\delta G$ throughout the domain I, requires either the extension of g to a slightly bigger interval $[-p\delta, 1+p\delta]$ or the consideration of the mollified function restricted to the subinterval $[p\delta, 1-p\delta]$. Our approach here is the first one. We seek an extension of g, g^*, which is constant on both intervals $[-p\delta, 0]$ and $[1, 1+p\delta]$, satisfying the conditions,

$$\|J_\delta g^* - g\|_{L^2[0,p\delta]} \text{ is minimum}$$

and

$$\|J_\delta g^* - g\|_{L^2[1-p\delta,1]} \text{ is minimum.}$$

The unique solution to this optimization problem at the point $t = 1$ is given by

$$g^* = \frac{\int_{1-p\delta}^{1}\left[g(t) - \int_0^1 \rho_\delta(t-s)\, g(s)\, ds\right]\left[\int_1^{1+p\delta} \rho_\delta(t-s)\, ds\right] dt}{\int_{1-p\delta}^{1}\left[\int_1^{1+p\delta} \rho_\delta(t-s)\, ds\right]^2 dt}.$$

A similar result holds at the end point $t = 0$. A proof of these statements can be found in [12].

For each $\delta > 0$, the extended function is defined on the interval $[-p\delta, 1 + p\delta]$ and the corresponding mollified function is computed on I.

4.4.2. Selection of parameters

The computation of the discrete mollified data vector,

$$G_\delta^\epsilon \equiv \left[J_\delta G^\epsilon(t_1), J_\delta G^\epsilon(t_2), \dots, J_\delta G^\epsilon(t_n)\right]^\top,$$

from the noisy data vector $G^\epsilon = \left[G_1^\epsilon, \dots, G_n^\epsilon\right]^\top$ requires the addition of

$$\eta = \left[p\frac{\delta}{\Delta t}\right] + 1$$

constant values, $\{\gamma_i\}_{i=1}^{\eta}$, $\gamma_i = \gamma$ and $\{\beta_i\}_{i=1}^{\eta}$, $\beta_i = \beta$, $i = 1, 2, \dots, \eta$, as follows,

$$G_{\text{ext}}^\epsilon = \left[\gamma_1, \gamma_2, \dots, \gamma_{\eta-1}, \gamma_\eta, G_1^\epsilon, G_2^\epsilon, \dots, G_{n-1}^\epsilon, G_n^\epsilon, \beta_1, \beta_2, \dots, \beta_{\eta-1}, \beta_\eta\right]^\top.$$

Now define the $n \times (n + 2r)$ circulant matrix A_δ where the first row is given by

$$(A_\delta)_{1j} = \begin{cases} \int_{s_{j-1}}^{s_j} \rho_\delta(-s)\, ds, & j = 1, 2, \dots, n, \\ 0, & j = n+1, \dots, n + 2\eta. \end{cases}$$

Then,

$$A_\delta G_{\text{ext}}^\epsilon = G_\delta^\epsilon.$$

We observe that the mollified data vector requires the computation of n inner products. Since the noise in the data is not known, an appropriate mollification parameter, introducing the correct degree of smoothing, should be selected. Such a parameter is determined by the principle of generalized cross validation, [13], as the value of δ that minimizes the functional,

$$\frac{\left(G_{\text{ext}}^\epsilon\right)^\top \left(I^\top - A_\delta^\top\right)(I - A_\delta)\, G_{\text{ext}}^\epsilon}{\operatorname{Trace}\left[\left(I^\top - A_\delta^\top\right)(I - A_\delta)\right]},$$

where the $n \times (n + 2\eta)$ matrix I has entries,

$$I_{ij} = \begin{cases} 1, & i = j, \quad i = 1, 2, \dots n, \\ 0, & \text{otherwise.} \end{cases}$$

We note that for fixed Δt, the data extension procedure dynamically updates the dimensions of all the vectors involved which depend on δ and also that the denominator of the GCV functional can be evaluated explicitly for each $\delta > 0$.

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